Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1615lxc

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	May 10	PROUSDDR now available on STN
NEWS 4	May 19	PROUSDDR: One FREE connect hour, per account, in both May and June 2004
NEWS 5	May 12	EXTEND option available in structure searching
NEWS 6	May 12	Polymer links for the POLYLINK command completed in REGISTRY
NEWS 7	May 17	FRFULL now available on STN
NEWS 8	May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
NEWS 9	May 27	CAplus super roles and document types searchable in REGISTRY
NEWS 10	May 27	Explore APOLLIT with free connect time in June 2004
NEWS 11	Jun 22	STN Patent Forums to be held July 19-22, 2004

NEWS EXPRESS	MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 19:08:59 ON 24 JUN 2004

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CAPLUS' ENTERED AT 19:09:29 ON 24 JUN 2004

FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26
FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

```
=> s (unattached or uncomplex or non-complexed or free or unbound) (2a) cyclodextrin
           903 UNATTACHED
            15 UNCOMPLEX
            27 UNCOMPLEXES
            42 UNCOMPLEX
               (UNCOMPLEX OR UNCOMPLEXES)
        659167 NON
            33 NONS
        659193 NON
               (NON OR NONS)
         29733 COMPLEXED
           166 NON-COMPLEXED
               (NON(W)COMPLEXED)
       1149185 FREE
           567 FREES
       1149661 FREE
               (FREE OR FREES)
         10698 UNBOUND
             1 UNBOUNDS
         10698 UNBOUND
               (UNBOUND OR UNBOUNDS)
         25338 CYCLODEXTRIN
          8293 CYCLODEXTRINS
         26033 CYCLODEXTRIN
               (CYCLODEXTRIN OR CYCLODEXTRINS)
L1         137 (UNATTACHED OR UNCOMPLEX OR NON-COMPLEXED OR FREE OR UNBOUND)
               (2A) CYCLODEXTRIN

=> s l1 (p)  (surfactant or emulsifier or surface active)
        159739 SURFACTANT
        143359 SURFACTANTS
        202420 SURFACTANT
               (SURFACTANT OR SURFACTANTS)
         29947 EMULSIFIER
         18223 EMULSIFIERS
         38155 EMULSIFIER
               (EMULSIFIER OR EMULSIFIERS)
       1946087 SURFACE
        378056 SURFACES
       2100985 SURFACE
               (SURFACE OR SURFACES)
        828308 ACTIVE
           702 ACTIVES
        828705 ACTIVE
               (ACTIVE OR ACTIVES)
         30415 SURFACE ACTIVE
```

(SURFACE(W)ACTIVE)
L2 11 L1 (P) (SURFACTANT OR EMULSIFIER OR SURFACE ACTIVE)

=> d l11 ibib kwic 1-
L11 NOT FOUND
The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> y

L3 285707 Y

=> d l2 ibib kwic 1-
YOU HAVE REQUESTED DATA FROM 11 ANSWERS - CONTINUE? Y/(N):y

L2 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:132555 CAPLUS
DOCUMENT NUMBER: 140:327743
TITLE: Simple Surfactant-Free Route to Mesoporous Organic-Inorganic Hybrid Silicas Containing Covalently Bound Cyclodextrins
AUTHOR(S): Liu, Chunqing; Lambert, Joseph B.; Fu, Lei
CORPORATE SOURCE: Department of Chemistry and Department of Materials Science and Engineering, Northwestern University, Evanston, IL, 60208, USA
SOURCE: Journal of Organic Chemistry (2004), 69(6), 2213-2216
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
IT 7585-39-9DP, β-Cyclodextrin, reaction product with isocyanatopropyltriethoxysilane 24801-88-5DP, 3-Isocyanatopropyltriethoxysilane, reaction product with β-**cyclodextrin**
RL: NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(monomer; **surfactant-free** route for synthesis of mesoporous organic-inorg. hybrid silica modified with cyclodextrin unit)
IT 7631-86-9DP, Silica, modified with **cyclodextrin**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(**surfactant-free** route for synthesis of mesoporous organic-inorg. hybrid silica modified with cyclodextrin unit)

L2 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:892237 CAPLUS
DOCUMENT NUMBER: 139:369370
TITLE: Surfactant-free rinsable skin conditioning compositions containing oils and stabilizers and skin benefit agents
INVENTOR(S): Deckner, George Endel; Manchuso, Scott Edward; Monsueir, William Joseph; Rodriguez, Victor Ruben; Sine, Mark Richard
PATENT ASSIGNEE(S): The Procter & Gamble Company, USA
SOURCE: U.S. Pat. Appl. Publ., 14 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003211069	A1	20031113	US 2002-142217	20020509
US 2003211061	A1	20031113	US 2002-298891	20021118
US 6699488	B2	20040302		
WO 2003094866	A1	20031120	WO 2003-US14320	20030507

W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

WO 2003094867	A1	20031120	WO 2003-US14321	20030507

W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-142217 A1 20020509
US 2002-298891 A 20021118

IT 56-81-5, Glycerine, biological studies 57-88-5, Cholesterol, biological studies 57-88-5D, Cholesterol, derivs. 79-10-7D, Acrylic acid, derivs., copolymers 112-92-5, Stearyl alcohol 1314-13-2, Zinc oxide, biological studies 1314-23-4, Zirconium oxide, biological studies 1332-37-2, Iron oxide, biological studies 1344-28-1, Aluminum oxide, biological studies 1948-56-7D, Amino acrylic acid, derivs., copolymer with acrylate and polyethylene glycol alkyl itaconate 7631-86-9, Silica, biological studies 7748-27-8D, Vinyl isodecanoate, copolymer with acrylate 9002-86-2, Polyvinyl chloride 9002-88-4, Polyethylene 9003-07-0, Polypropylene 9003-53-6, Polystyrene 9006-65-9, Dimethicone 11129-18-3, Cerium oxide 11129-60-5, Manganese oxide 12619-70-4D, **Cyclodextrins**, derivs. 13463-67-7, Titanium oxide, biological studies 26446-35-5D, Acetoglyceride, esters 31692-79-2, Dimethiconol 36653-82-4, Cetyl alcohol 52352-43-9D, Steareth-20 methacrylate, copolymer with acrylate 80455-45-4, Cetyl hydroxyethyl cellulose 98616-25-2, Polyquaternium 24 115047-92-2D, Beheneth-25 methacrylate, copolymer with acrylate 152502-70-0D, alkyl ether, copolymer with acrylate and amino acrylate 204011-36-9D, copolymer with acrylate 233265-18-4, Aculyn 46 250241-42-0D, Steareth-20 itaconate, copolymer with acrylate
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(**surfactant-free** rinsable skin conditioning compns. containing oils and stabilizers and skin benefit agents)

L2 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:545298 CAPLUS
DOCUMENT NUMBER: 139:230916
TITLE: Heat Capacity Study to Evidence the Interactions between Cyclodextrin and Surfactant in the Monomeric and Micellized States

AUTHOR(S): De Lisi, R.; Lazzara, G.; Milioto, S.; Muratore, N.; Terekhova, I. V.
CORPORATE SOURCE: Dipartimento di Chimica Fisica F. Accascina, Universita di Palermo, Palermo, 90128, Italy
SOURCE: Langmuir (2003), 19(18), 7188-7195
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The heat capacities of transfer (ΔCpt) of hydroxypropyl-α-cyclodextrin and hydroxypropyl-γ-cyclodextrin (0.05 mol kg-1) from water to aqueous solns. of sodium hexanoate, sodium decanoate, and sodium dodecanoate were determined at 298 K. The measurements were extended to both the pre- and the post-micellar regions. The shape of the ΔCpt as a function of the **surfactant** concentration curve is system specific. As well, the ΔCpt magnitude depends on the macrocycle cavity being largely neg. for HP-γ-CD. The qual. anal. of the exptl. data highlights that the features of the heat capacity are different from those of the enthalpy due to the important effect of temperature on the equilibrium in solution The exptl. points were treated by means of a new equation based on the following contributions: (i) the formation of host-guest complexes in the aqueous phase, (ii) the shift of the micellization equilibrium induced by the cyclodextrin, and (iii) the interaction between micelle and **cyclodextrin** (**free** and complexed). The resulting equation is involved since it contains not only the terms related to the various equilibrium in solution but also those relative to their shift with temperature Despite its complexity, the equation fitted very well the exptl. points in the absence and the presence of micelles.

L2 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:898264 CAPLUS
DOCUMENT NUMBER: 138:90158
TITLE: Cyclodextrins in Polymer Synthesis: A Simple and Surfactant Free Way to Polymer Particles Having Narrow Particle Size Distribution
AUTHOR(S): Storsberg, Joachim; van Aert, Huub; van Roost, Christiaan; Ritter, Helmut
CORPORATE SOURCE: R&D Materials, Agfa-Gevaert N.V., Mortsel, B-2640, Belg.
SOURCE: Macromolecules (2003), 36(1), 50-53
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ST radical addn polymn **surfactant free** process **cyclodextrin** additive

L2 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:585827 CAPLUS
DOCUMENT NUMBER: 137:262738
TITLE: Thermodynamic Evidence of Cyclodextrin-Micelle Interactions
AUTHOR(S): De Lisi, R.; Milioto, S.; Muratore, N.
CORPORATE SOURCE: Dipartimento di Chimica Fisica, Universita di Palermo, Palermo, 90128, Italy
SOURCE: Journal of Physical Chemistry B (2002), 106(35),

8944-8953
CODEN: JPCBFK; ISSN: 1520-6106
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The enthalpy of transfer (ΔHt) of hydroxypropyl-α-cyclodextrin (HP-α-CD), hydroxypropyl-β-cyclodextrin (HP-β-CD), and β-cyclodextrin (β-CD) from water to the aqueous C6F13CO2Na and C7F15CO2Na solns. were determined in the pre- and post-micellar regions. The behavior of the macrocycles is system specific. Generally, the magnitude of the enthalpy is influenced by several factors: (1) the alkyl chain length of the **surfactant**, (2) the cyclodextrin cavity and its alkylation, (3) the interactions between the **free cyclodextrin** and the **free surfactant**, (4) the host-guest equilibrium constant, (5) the host/guest stoichiometry, and (6) the micelle-**cyclodextrin** (**free** and/or complexed) interactions. As far as the premicellar region is concerned, HP-α-CD does not form the host-guest complexes. β-CD and HP-β-CD in the aqueous C7F15CO2Na solns. form host-guest complexes of 1:1 stoichiometry; β-CD shows a larger binding affinity toward the **surfactant** as a compensative effect between the more neg. enthalpy and entropy. Besides 1:1 complexes, HP-β-CD in aqueous C6F13CO2Na solns. forms complexes of 1:2 stoichiometry (1 cyclodextrin:2 **surfactants**). Their presence was evidenced by the min. in the ΔHt vs the **surfactant** concentration (fSmS) trend. The equation derived to take into account both 1:1 and 1:2 complexes equilibrium was successfully applied to the present data and those of HP-α-CD/sodium alkanoate systems previously studied by us. As far as the postmicellar region is concerned, HP-α-CD was treated like an additive, which distributes between the aqueous and the micellar phases. An equation was proposed to rationalize the enthalpy data dealing with the cyclodextrins exhibiting inclusion complex formation. It was based on the following phenomena: (1) formation of 1:1 and 1:2 complexes in the aqueous phase, (2) distribution of **free cyclodextrin**, 1:1 complex, and 1:2 complex between the aqueous and the micellar phases, and (3) shift of the micellization equilibrium induced by the cyclodextrin. As a general feature, **cyclodextrin** (**free** and/or complexed) shows affinity toward the micelles because of the favorable interactions between the carboxylate head in the hydrophilic shell and the hydroxyl groups of the cyclodextrin. C6F13CO2Na micelles compared to C7F15CO2Na exhibit a slightly larger affinity toward HP-α-CD controlled by more neg. enthalpy and entropy changes. A single mechanism governs the interaction between the C7F15CO2Na micelles and the 1:1 complexes of HP-β-CD/ **surfactant** and β-CD/ **surfactant**, as the standard free energy, enthalpy, and entropy of transfer of the two complexes from the aqueous to the micellar phases are identical. The 1:2 complex (1 HP-β-CD:2 C6F13CO2Na) weakly binds to the micelles according to the unfavorable interactions between the micellar surface and the doubly charged complex.

L2 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:143878 CAPLUS
DOCUMENT NUMBER: 136:156229
TITLE: Improved toothpaste composition
INVENTOR(S): Kim, Hu Deok
PATENT ASSIGNEE(S): LG Chemical Co., Ltd., S. Korea
SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given
CODEN: KRXXA7
DOCUMENT TYPE: Patent
LANGUAGE: Korean
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2000039602	A	20000705	KR 1998-54992	19981215

PRIORITY APPLN. INFO.: KR 1998-54992 19981215

ST toothpaste **cyclodextrin surfactant** irritation **free**

L2 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:760240 CAPLUS
DOCUMENT NUMBER: 134:30623
TITLE: β-cyclodextrin-micelle mixed systems as a reaction medium. Denitrosation of N-methyl-N-nitroso-p-toluene-sulfonamide
AUTHOR(S): Fernandez, I.; Garcia-Rio, L.; Herves, P.; Mejuto, J. C.; Perez-Juste, J.; Rodriguez-Dafonte, P.
CORPORATE SOURCE: Departamento de Quimica Fisica, Facultad de Ciencias, Universidad de Vigo, Vigo, Spain
SOURCE: Journal of Physical Organic Chemistry (2000), 13(10), 664-669
CODEN: JPOCEE; ISSN: 0894-3230
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The kinetics of the acid hydrolysis of N-methyl-N-nitroso-p-toluenesulfonamide (MNTS) were studied in media containing different cationic micellar aggregates (lauryltrimethylammonium bromide, tetradecyltrimethylammonium bromide and cetyltrimethylammonium chloride) and β-cyclodextrin (β-CD). The results were interpreted in terms of the pseudo-phase model. The model takes into account the formation of both β-CD- **surfactant** and β-CD-MNTS complexes. The presence of β-CD has no effect on existing micelles but raises the cmc. Complexation of **surfactant** by β-CD makes the cmc dependent on β-CD concentration because the cmc is now the sum of the concns. of free and complexed **surfactant** when micelles begin to form. At **surfactant** concns. above the cmc, competition between the micellization and complexation processes leads to the existence of a significant concentration of **free cyclodextrin** .

L2 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:190723 CAPLUS
DOCUMENT NUMBER: 132:227182
TITLE: Emulsifier-free finely dispersed systems of the oil-in-water or water-in-oil type
INVENTOR(S): Gers-Barlag, Heinrich; Mueller, Anja
PATENT ASSIGNEE(S): Beiersdorf Aktiengesellschaft, Germany
SOURCE: Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 987007	A2	20000322	EP 1999-116875	19990906
EP 987007	A3	20011031		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
DE 19842766	A1	20000323	DE 1998-19842766	19980918

US 6428796	B1	20020806	US 1999-388601	19990902
US 2002110570	A1	20020815		
JP 2000095637	A2	20000404	JP 1999-259170	19990913
US 2003003122	A1	20030102	US 2002-132749	20020425
US 6703032	B2	20040309		

PRIORITY APPLN. INFO.: DE 1998-19842766 A 19980918
US 1999-388601 A3 19990902

IT 7585-39-9, β- **Cyclodextrin** 12619-70-4, **Cyclodextrin** 17465-86-0, γ- **Cyclodextrin**
RL: BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(stabilizer; **emulsifier-free** finely dispersed oil-in-water or water-in-oil systems)

L2 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:619827 CAPLUS
DOCUMENT NUMBER: 131:351570
TITLE: Basic hydrolysis of substituted nitrophenyl acetates in β-cyclodextrin/ **surfactant** mixed systems. Evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**
AUTHOR(S): Alvarez, A. R.; Garcia-Rio, L.; Herves, P.; Leis, J. R.; Mejuto, J. C.; Perez-Juste, J.
CORPORATE SOURCE: Departamento de Quimica Fisica Facultad de Quimica, Universidad de Santiago, Santiago de Compostela, E-15706, Spain
SOURCE: Langmuir (1999), 15(24), 8368-8375
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TI Basic hydrolysis of substituted nitrophenyl acetates in β-cyclodextrin/ **surfactant** mixed systems. Evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**

IT Hydrolysis
Hydrolysis catalysts
Micelles
Surfactants
(basic hydrolysis of substituted nitrophenyl acetates in cyclodextrin **surfactant** mixed systems and evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**)

IT 7585-39-9, β-Cyclodextrin
RL: CAT (Catalyst use); USES (Uses)
(basic hydrolysis of substituted nitrophenyl acetates in β-cyclodextrin **surfactant** mixed systems and evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**)

IT 151-21-3, Sodium dodecyl sulfate, reactions 610-69-5, o-Nitrophenyl acetate 830-03-5, p-Nitrophenyl acetate 1119-97-7, Tetradecyltrimethylammonium bromide 1523-06-4 84927-25-3, Tetradecyltrimethylammonium hydroxide
RL: RCT (Reactant); RACT (Reactant or reagent)
(basic hydrolysis of substituted nitrophenyl acetates in β-cyclodextrin **surfactant** mixed systems and evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**)

L2 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:558907 CAPLUS

DOCUMENT NUMBER: 127:220309
TITLE: Investigation of Micellar Media Containing β-Cyclodextrins by Means of Reaction Kinetics: Basic Hydrolysis of N-Methyl-N-nitroso-p-toluenesulfonamide
AUTHOR(S): Garcia-Rio, L.; Leis, J. R.; Mejuto, J. C.; Perez-Juste, J.
CORPORATE SOURCE: Departamento de Quimica Fisica Facultad de Quimica, Universidad de Santiago, Santiago, 15706, Spain
SOURCE: Journal of Physical Chemistry B (1997), 101(38), 7383-7389
CODEN: JPCBFK; ISSN: 1089-5647
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The kinetics of the basic hydrolysis of N-methyl-N-nitroso-p-toluenesulfonamide were studied in media containing sodium dodecyl sulfate (SDS) or tetradecyltrimethylammonium bromide (TTABr) micelles and β-cyclodextrin (CD). Under the exptl. conditions, [NaOH] = 0.17 M, all CD will have been deprotonated; thus, binding consts. apply to the CD anion. The results have been interpreted in terms of a pseudophase model that takes into account the formation of both CD-**surfactant** and CD-substrate complexes and also, for TTABr systems, the exchange of Br- and OH- ions between the micellar and aqueous pseudophases. The presence of CD has no effect on existing SDS or TTABr micelles but raises the cmc: complexation of **surfactant** by cyclodextrin makes the cmc dependent on CD concentration because the cmc is now the sum of the concns. of free and complexed **surfactant** when micelles begin to form; increasing [CD] reduces the former quantity but increases the latter to a greater extent. At **surfactant** concns. above the cmc, competition between the micellization and complexation processes leads to the existence of a significant concentration of **free cyclodextrin**.

L2 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:428661 CAPLUS
DOCUMENT NUMBER: 127:55655
TITLE: Stable emulsions and topical preparations containing α-cyclodextrin and polyoxyethylene glycol
INVENTOR(S): Kaminuma, Mikiko; Nakajima, Hideo
PATENT ASSIGNEE(S): Shiseido Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09124437	A2	19970513	JP 1995-306811	19951031

PRIORITY APPLN. INFO.: JP 1995-306811 19951031

IT 57-11-4, Octadecanoic acid, biological studies 110-27-0, Isopropyl myristate 111-01-3, Squalane 112-80-1, Oleic acid, biological studies 9016-00-6, Dimethyl siloxane 10016-20-3, α- **Cyclodextrin** 25322-68-3 26086-33-9 31900-57-9, Dimethylsilanediol homopolymer 36653-82-4, Cetyl alcohol 59130-69-7, Cetyl 2-ethylhexanoate 72585-97-8, Cetyl isooctanoate
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(stable **surfactant-free** emulsions containing α-cyclodextrin, polyoxyethylene glycol, and oils for skin and hair cosmetics)

```
=> s (unattached or uncomplex or non-complexed or free or unbound) (a) cyclodextrin
           903 UNATTACHED
            15 UNCOMPLEX
            27 UNCOMPLEXES
            42 UNCOMPLEX
                 (UNCOMPLEX OR UNCOMPLEXES)
        659167 NON
            33 NONS
        659193 NON
                 (NON OR NONS)
         29733 COMPLEXED
           166 NON-COMPLEXED
                 (NON(W)COMPLEXED)
       1149185 FREE
           567 FREES
       1149661 FREE
                 (FREE OR FREES)
         10698 UNBOUND
             1 UNBOUNDS
         10698 UNBOUND
                 (UNBOUND OR UNBOUNDS)
         25338 CYCLODEXTRIN
          8293 CYCLODEXTRINS
         26033 CYCLODEXTRIN
                 (CYCLODEXTRIN OR CYCLODEXTRINS)
L4           32 (UNATTACHED OR UNCOMPLEX OR NON-COMPLEXED OR FREE OR UNBOUND)
              (A) CYCLODEXTRIN

=> s l4 (p)  (surfactant or emulsifier or surface active)
        159739 SURFACTANT
        143359 SURFACTANTS
        202420 SURFACTANT
                 (SURFACTANT OR SURFACTANTS)
         29947 EMULSIFIER
         18223 EMULSIFIERS
         38155 EMULSIFIER
                 (EMULSIFIER OR EMULSIFIERS)
       1946087 SURFACE
        378056 SURFACES
       2100985 SURFACE
                 (SURFACE OR SURFACES)
        828308 ACTIVE
           702 ACTIVES
        828705 ACTIVE
                 (ACTIVE OR ACTIVES)
         30415 SURFACE ACTIVE
                 (SURFACE(W)ACTIVE)
L5            5 L4 (P)  (SURFACTANT OR EMULSIFIER OR SURFACE ACTIVE)

=> d l5 ibib kwic 1-
YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y


L5   ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2003:545298  CAPLUS
DOCUMENT NUMBER:          139:230916
TITLE:                    Heat Capacity Study to Evidence the Interactions
                          between Cyclodextrin and Surfactant in the Monomeric
                          and Micellized States
AUTHOR(S):                De Lisi, R.; Lazzara, G.; Milioto, S.; Muratore, N.;
                          Terekhova, I. V.
```

CORPORATE SOURCE: Dipartimento di Chimica Fisica F. Accascina, Universita di Palermo, Palermo, 90128, Italy
SOURCE: Langmuir (2003), 19(18), 7188-7195
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The heat capacities of transfer (ΔCpt) of hydroxypropyl-α-cyclodextrin and hydroxypropyl-γ-cyclodextrin (0.05 mol kg-1) from water to aqueous solns. of sodium hexanoate, sodium decanoate, and sodium dodecanoate were determined at 298 K. The measurements were extended to both the pre- and the post-micellar regions. The shape of the ΔCpt as a function of the **surfactant** concentration curve is system specific. As well, the ΔCpt magnitude depends on the macrocycle cavity being largely neg. for HP-γ-CD. The qual. anal. of the exptl. data highlights that the features of the heat capacity are different from those of the enthalpy due to the important effect of temperature on the equilibrium in solution The exptl. points were treated by means of a new equation based on the following contributions: (i) the formation of host-guest complexes in the aqueous phase, (ii) the shift of the micellization equilibrium induced by the cyclodextrin, and (iii) the interaction between micelle and **cyclodextrin** (**free** and complexed). The resulting equation is involved since it contains not only the terms related to the various equilibrium in solution but also those relative to their shift with temperature Despite its complexity, the equation fitted very well the exptl. points in the absence and the presence of micelles.

L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:585827 CAPLUS
DOCUMENT NUMBER: 137:262738
TITLE: Thermodynamic Evidence of Cyclodextrin-Micelle Interactions
AUTHOR(S): De Lisi, R.; Milioto, S.; Muratore, N.
CORPORATE SOURCE: Dipartimento di Chimica Fisica, Universita di Palermo, Palermo, 90128, Italy
SOURCE: Journal of Physical Chemistry B (2002), 106(35), 8944-8953
CODEN: JPCBFK; ISSN: 1520-6106
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The enthalpy of transfer (ΔHt) of hydroxypropyl-α-cyclodextrin (HP-α-CD), hydroxypropyl-β-cyclodextrin (HP-β-CD), and β-cyclodextrin (β-CD) from water to the aqueous C6F13CO2Na and C7F15CO2Na solns. were determined in the pre- and post-micellar regions. The behavior of the macrocycles is system specific. Generally, the magnitude of the enthalpy is influenced by several factors: (1) the alkyl chain length of the **surfactant**, (2) the cyclodextrin cavity and its alkylation, (3) the interactions between the **free** **cyclodextrin** and the free **surfactant**, (4) the host-guest equilibrium constant, (5) the host/guest stoichiometry, and (6) the micelle-**cyclodextrin** (**free** and/or complexed) interactions. As far as the premicellar region is concerned, HP-α-CD does not form the host-guest complexes. β-CD and HP-β-CD in the aqueous C7F15CO2Na solns. form host-guest complexes of 1:1 stoichiometry; β-CD shows a larger binding affinity toward the **surfactant**

as a compensative effect between the more neg. enthalpy and entropy. Besides 1:1 complexes, HP-β-CD in aqueous C6F13CO2Na solns. forms complexes of 1:2 stoichiometry (1 cyclodextrin:2 **surfactants**). Their presence was evidenced by the min. in the ΔHt vs the **surfactant** concentration (fSmS) trend. The equation derived to take into account both 1:1 and 1:2 complexes equilibrium was successfully applied to the present data and those of HP-α-CD/sodium alkanoate systems previously studied by us. As far as the postmicellar region is concerned, HP-α-CD was treated like an additive, which distributes between the aqueous and the micellar phases. An equation was proposed to rationalize the enthalpy data dealing with the cyclodextrins exhibiting inclusion complex formation. It was based on the following phenomena: (1) formation of 1:1 and 1:2 complexes in the aqueous phase, (2) distribution of **free cyclodextrin**, 1:1 complex, and 1:2 complex between the aqueous and the micellar phases, and (3) shift of the micellization equilibrium induced by the cyclodextrin. As a general feature, **cyclodextrin** (**free** and/or complexed) shows affinity toward the micelles because of the favorable interactions between the carboxylate head in the hydrophilic shell and the hydroxyl groups of the cyclodextrin. C6F13CO2Na micelles compared to C7F15CO2Na exhibit a slightly larger affinity toward HP-α-CD controlled by more neg. enthalpy and entropy changes. A single mechanism governs the interaction between the C7F15CO2Na micelles and the 1:1 complexes of HP-β-CD/ **surfactant** and β-CD/ **surfactant**, as the standard free energy, enthalpy, and entropy of transfer of the two complexes from the aqueous to the micellar phases are identical. The 1:2 complex (1 HP-β-CD:2 C6F13CO2Na) weakly binds to the micelles according to the unfavorable interactions between the micellar surface and the doubly charged complex.

L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:760240 CAPLUS
DOCUMENT NUMBER: 134:30623
TITLE: β-cyclodextrin-micelle mixed systems as a reaction medium. Denitrosation of N-methyl-N-nitroso-p-toluene-sulfonamide
AUTHOR(S): Fernandez, I.; Garcia-Rio, L.; Herves, P.; Mejuto, J. C.; Perez-Juste, J.; Rodriguez-Dafonte, P.
CORPORATE SOURCE: Departamento de Quimica Fisica, Facultad de Ciencias, Universidad de Vigo, Vigo, Spain
SOURCE: Journal of Physical Organic Chemistry (2000), 13(10), 664-669
CODEN: JPOCEE; ISSN: 0894-3230
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The kinetics of the acid hydrolysis of N-methyl-N-nitroso-p-toluenesulfonamide (MNTS) were studied in media containing different cationic micellar aggregates (lauryltrimethylammonium bromide, tetradecyltrimethylammonium bromide and cetyltrimethylammonium chloride) and β-cyclodextrin (β-CD). The results were interpreted in terms of the pseudo-phase model. The model takes into account the formation of both β-CD- **surfactant** and β-CD-MNTS complexes. The presence of β-CD has no effect on existing micelles but raises the cmc. Complexation of **surfactant** by β-CD makes the cmc dependent on β-CD concentration because the cmc is now the sum of the concns. of free and complexed **surfactant** when micelles begin to form. At **surfactant** concns. above the cmc, competition between the micellization and complexation processes leads to the existence of a significant concentration of **free cyclodextrin**
.

L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:619827 CAPLUS
DOCUMENT NUMBER: 131:351570
TITLE: Basic hydrolysis of substituted nitrophenyl acetates in β-cyclodextrin/ **surfactant** mixed systems. Evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**
AUTHOR(S): Alvarez, A. R.; Garcia-Rio, L.; Herves, P.; Leis, J. R.; Mejuto, J. C.; Perez-Juste, J.
CORPORATE SOURCE: Departamento de Quimica Fisica Facultad de Quimica, Universidad de Santiago, Santiago de Compostela, E-15706, Spain
SOURCE: Langmuir (1999), 15(24), 8368-8375
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TI Basic hydrolysis of substituted nitrophenyl acetates in β-cyclodextrin/ **surfactant** mixed systems. Evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**

IT Hydrolysis
Hydrolysis catalysts
Micelles
Surfactants
(basic hydrolysis of substituted nitrophenyl acetates in cyclodextrin **surfactant** mixed systems and evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**)

IT 7585-39-9, β-Cyclodextrin
RL: CAT (Catalyst use); USES (Uses)
(basic hydrolysis of substituted nitrophenyl acetates in β-cyclodextrin **surfactant** mixed systems and evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**)

IT 151-21-3, Sodium dodecyl sulfate, reactions 610-69-5, o-Nitrophenyl acetate 830-03-5, p-Nitrophenyl acetate 1119-97-7, Tetradecyltrimethylammonium bromide 1523-06-4 84927-25-3, Tetradecyltrimethylammonium hydroxide
RL: RCT (Reactant); RACT (Reactant or reagent)
(basic hydrolysis of substituted nitrophenyl acetates in β-cyclodextrin **surfactant** mixed systems and evidence of **free cyclodextrin** in equilibrium with micellized **surfactant**)

L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:558907 CAPLUS
DOCUMENT NUMBER: 127:220309
TITLE: Investigation of Micellar Media Containing β-Cyclodextrins by Means of Reaction Kinetics: Basic Hydrolysis of N-Methyl-N-nitroso-p-toluenesulfonamide
AUTHOR(S): Garcia-Rio, L.; Leis, J. R.; Mejuto, J. C.; Perez-Juste, J.
CORPORATE SOURCE: Departamento de Quimica Fisica Facultad de Quimica, Universidad de Santiago, Santiago, 15706, Spain
SOURCE: Journal of Physical Chemistry B (1997), 101(38), 7383-7389
CODEN: JPCBFK; ISSN: 1089-5647
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The kinetics of the basic hydrolysis of N-methyl-N-nitroso-p-toluenesulfonamide were studied in media containing sodium dodecyl sulfate (SDS) or tetradecyltrimethylammonium bromide (TTABr) micelles and β-cyclodextrin (CD). Under the exptl. conditions, [NaOH] = 0.17 M, all CD will have been deprotonated; thus, binding consts. apply to the CD anion. The results have been interpreted in terms of a pseudophase model that takes into account the formation of both CD-**surfactant** and CD-substrate complexes and also, for TTABr systems, the exchange of Br- and OH- ions between the micellar and aqueous pseudophases. The presence of CD has no effect on existing SDS or TTABr micelles but raises the cmc: complexation of **surfactant** by cyclodextrin makes the cmc dependent on CD concentration because the cmc is now the sum of the concns. of free and complexed **surfactant** when micelles begin to form; increasing [CD] reduces the former quantity but increases the latter to a greater extent. At **surfactant** concns. above the cmc, competition between the micellization and complexation processes leads to the existence of a significant concentration of **free cyclodextrin**.

```
=> s functional (2a) cyclodextrin
        432609 FUNCTIONAL
          3483 FUNCTIONALS
        433595 FUNCTIONAL
                 (FUNCTIONAL OR FUNCTIONALS)
         25338 CYCLODEXTRIN
          8293 CYCLODEXTRINS
         26033 CYCLODEXTRIN
                 (CYCLODEXTRIN OR CYCLODEXTRINS)
L6          78 FUNCTIONAL (2A) CYCLODEXTRIN

=> s functional (2a) cyclodextrin (3a) (free or unbound or uncomplexed or
unattached)
        432609 FUNCTIONAL
          3483 FUNCTIONALS
        433595 FUNCTIONAL
                 (FUNCTIONAL OR FUNCTIONALS)
         25338 CYCLODEXTRIN
          8293 CYCLODEXTRINS
         26033 CYCLODEXTRIN
                 (CYCLODEXTRIN OR CYCLODEXTRINS)
       1149185 FREE
           567 FREES
       1149661 FREE
                 (FREE OR FREES)
         10698 UNBOUND
             1 UNBOUNDS
         10698 UNBOUND
                 (UNBOUND OR UNBOUNDS)
          3282 UNCOMPLEXED
           903 UNATTACHED
L7            0 FUNCTIONAL (2A) CYCLODEXTRIN (3A) (FREE OR UNBOUND OR UNCOMPLEXE
              D OR UNATTACHED)

=> s functional (2a) cyclodextrin (p) (free or unbound or uncomplexed or unattached)
        432609 FUNCTIONAL
          3483 FUNCTIONALS
        433595 FUNCTIONAL
                 (FUNCTIONAL OR FUNCTIONALS)
         25338 CYCLODEXTRIN
          8293 CYCLODEXTRINS
         26033 CYCLODEXTRIN
```

```
                (CYCLODEXTRIN OR CYCLODEXTRINS)
       1149185 FREE
           567 FREES
       1149661 FREE
                (FREE OR FREES)
         10698 UNBOUND
             1 UNBOUNDS
         10698 UNBOUND
                (UNBOUND OR UNBOUNDS)
          3282 UNCOMPLEXED
           903 UNATTACHED
L8            0 FUNCTIONAL (2A) CYCLODEXTRIN (P) (FREE OR UNBOUND OR UNCOMPLEXED
                OR UNATTACHED)

=> s functional (2a) cyclodextrin (p) (surfactant or emulsifier or surface active)
        432609 FUNCTIONAL
          3483 FUNCTIONALS
        433595 FUNCTIONAL
                (FUNCTIONAL OR FUNCTIONALS)
         25338 CYCLODEXTRIN
          8293 CYCLODEXTRINS
         26033 CYCLODEXTRIN
                (CYCLODEXTRIN OR CYCLODEXTRINS)
        159739 SURFACTANT
        143359 SURFACTANTS
        202420 SURFACTANT
                (SURFACTANT OR SURFACTANTS)
         29947 EMULSIFIER
         18223 EMULSIFIERS
         38155 EMULSIFIER
                (EMULSIFIER OR EMULSIFIERS)
       1946087 SURFACE
        378056 SURFACES
       2100985 SURFACE
                (SURFACE OR SURFACES)
        828308 ACTIVE
           702 ACTIVES
        828705 ACTIVE
                (ACTIVE OR ACTIVES)
         30415 SURFACE ACTIVE
                (SURFACE(W)ACTIVE)
L9            2 FUNCTIONAL (2A) CYCLODEXTRIN (P) (SURFACTANT OR EMULSIFIER OR
                SURFACE ACTIVE)

=> s functional (2a) cyclodextrin (p) (surfactant or tenside or emulsifier or
surface active)
        432609 FUNCTIONAL
          3483 FUNCTIONALS
        433595 FUNCTIONAL
                (FUNCTIONAL OR FUNCTIONALS)
         25338 CYCLODEXTRIN
          8293 CYCLODEXTRINS
         26033 CYCLODEXTRIN
                (CYCLODEXTRIN OR CYCLODEXTRINS)
        159739 SURFACTANT
        143359 SURFACTANTS
        202420 SURFACTANT
                (SURFACTANT OR SURFACTANTS)
           557 TENSIDE
           526 TENSIDES
           910 TENSIDE
                (TENSIDE OR TENSIDES)
         29947 EMULSIFIER
```

```
         18223 EMULSIFIERS
         38155 EMULSIFIER
                 (EMULSIFIER OR EMULSIFIERS)
       1946087 SURFACE
        378056 SURFACES
       2100985 SURFACE
                 (SURFACE OR SURFACES)
        828308 ACTIVE
           702 ACTIVES
        828705 ACTIVE
                 (ACTIVE OR ACTIVES)
         30415 SURFACE ACTIVE
                 (SURFACE(W)ACTIVE)
L10          2 FUNCTIONAL (2A) CYCLODEXTRIN (P) (SURFACTANT OR TENSIDE OR EMULS
               IFIER OR SURFACE ACTIVE)

=> d l9 ibib kwic 1-
YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

L9   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:        2004:356124  CAPLUS
TITLE:                   Self-association of cyclodextrins and cyclodextrin
                         complexes
AUTHOR(S):               Loftsson, Thorsteinn; Masson, Mar; Brewster, Marcus E.
CORPORATE SOURCE:        Faculty of Pharmacy, University of Iceland, Reykjavik,
                         IS-107, Iceland
SOURCE:                  Journal of Pharmaceutical Sciences (2004), 93(5),
                         1091-1099
                         CODEN: JPMSAE; ISSN: 0022-3549
PUBLISHER:               Wiley-Liss, Inc.
DOCUMENT TYPE:           Journal
LANGUAGE:                English
REFERENCE COUNT:         57    THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
AB   Cyclodextrins are useful functional excipients, which
     are being used in an ever-increasing way to camouflage undesirable
     pharmaceutical characteristics, especially poor aqueous solubility  It has
generally been
     assumed that the mechanism whereby cyclodextrins exert their effects,
especially
     their augmentation of solubility, is via the formation of noncovalent, dynamic
     inclusion complexes.  This is a model, which regards drug-cyclodextrin
     interactions as a discrete phenomenon and ignores the possible interaction
     of these complexes with one another.  It is becoming increasingly apparent
     that such assumptions may not be universally applicable or all
     encompassing.  Specifically, there is a growing body of evidence that
     supports the important contribution of non-inclusion-based aspects for
     drug solubilization by cyclodextrins including surfactant-like
     effects and mol. aggregation.  This short review attempts to assess the
     available literature for areas in which such non-inclusion mechanisms are
     apparent and tries to interpret these in the context of a broader working
     theory as to how cyclodextrins exert their beneficial effects.

L9   ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:        1988:434512  CAPLUS
DOCUMENT NUMBER:         109:34512
TITLE:                   Studies on functional properties and applications of
                         β-cyclodextrin. 1. Emulsification, reduction of
                         bitterness, hygroscopicity and foaming
AUTHOR(S):               Chiu, C. P.; Lin, T. C.; Cheng, S. W.; Chuang, W. L.
CORPORATE SOURCE:        Dep. Nutr. Food Sci., Fn Jen Univ., Taiwan
SOURCE:                  Jiemian Kexue Huizhi (1988), 11(1), 38-44
                         CODEN: CMKCEW; ISSN: 1026-325X
```

DOCUMENT TYPE: Journal
LANGUAGE: Chinese
ST **cyclodextrin functional** property application; **emulsifier** cyclodextrin; hygroscopicity cyclodextrin; foaming cyclodextrin; bitterness redn cyclodextrin

=> d l9 ibib kwic 2

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:434512 CAPLUS
DOCUMENT NUMBER: 109:34512
TITLE: Studies on functional properties and applications of β-cyclodextrin. 1. Emulsification, reduction of bitterness, hygroscopicity and foaming
AUTHOR(S): Chiu, C. P.; Lin, T. C.; Cheng, S. W.; Chuang, W. L.
CORPORATE SOURCE: Dep. Nutr. Food Sci., Fn Jen Univ., Taiwan
SOURCE: Jiemian Kexue Huizhi (1988), 11(1), 38-44
CODEN: CMKCEW; ISSN: 1026-325X
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
ST **cyclodextrin functional** property application; **emulsifier** cyclodextrin; hygroscopicity cyclodextrin; foaming cyclodextrin; bitterness redn cyclodextrin

=> d his full

(FILE 'HOME' ENTERED AT 19:08:59 ON 24 JUN 2004)

FILE 'CAPLUS' ENTERED AT 19:09:29 ON 24 JUN 2004
L1 137 SEA ABB=ON PLU=ON (UNATTACHED OR UNCOMPLEX OR NON-COMPLEXED OR FREE OR UNBOUND) (2A) CYCLODEXTRIN
L2 11 SEA ABB=ON PLU=ON L1 (P) (SURFACTANT OR EMULSIFIER OR SURFACE ACTIVE)
L3 285707 SEA ABB=ON PLU=ON Y
D L2 IBIB KWIC 1-
L4 32 SEA ABB=ON PLU=ON (UNATTACHED OR UNCOMPLEX OR NON-COMPLEXED OR FREE OR UNBOUND) (A) CYCLODEXTRIN
L5 5 SEA ABB=ON PLU=ON L4 (P) (SURFACTANT OR EMULSIFIER OR SURFACE ACTIVE)
D L5 IBIB KWIC 1-
L6 78 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN
L7 0 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN (3A) (FREE OR UNBOUND OR UNCOMPLEXED OR UNATTACHED)
L8 0 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN (P) (FREE OR UNBOUND OR UNCOMPLEXED OR UNATTACHED)
L9 2 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN (P) (SURFACTAN T OR EMULSIFIER OR SURFACE ACTIVE)
L10 2 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN (P) (SURFACTAN T OR TENSIDE OR EMULSIFIER OR SURFACE ACTIVE)
D L9 IBIB KWIC 1-
D L9 IBIB KWIC 2

FILE HOME

FILE CAPLUS

FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26
FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

```
=> s functional (2a) cyclodextrin and (surfactant or tenside or emulsifier or
surface active)
        432609 FUNCTIONAL
          3483 FUNCTIONALS
        433595 FUNCTIONAL
                 (FUNCTIONAL OR FUNCTIONALS)
         25338 CYCLODEXTRIN
          8293 CYCLODEXTRINS
         26033 CYCLODEXTRIN
                 (CYCLODEXTRIN OR CYCLODEXTRINS)
            78 FUNCTIONAL (2A) CYCLODEXTRIN
        159739 SURFACTANT
        143359 SURFACTANTS
        202420 SURFACTANT
                 (SURFACTANT OR SURFACTANTS)
           557 TENSIDE
           526 TENSIDES
           910 TENSIDE
                 (TENSIDE OR TENSIDES)
         29947 EMULSIFIER
         18223 EMULSIFIERS
         38155 EMULSIFIER
                 (EMULSIFIER OR EMULSIFIERS)
       1946087 SURFACE
        378056 SURFACES
       2100985 SURFACE
                 (SURFACE OR SURFACES)
        828308 ACTIVE
           702 ACTIVES
        828705 ACTIVE
                 (ACTIVE OR ACTIVES)
         30415 SURFACE ACTIVE
                 (SURFACE(W)ACTIVE)
L11           3 FUNCTIONAL (2A) CYCLODEXTRIN AND (SURFACTANT OR TENSIDE OR EMULS
                IFIER OR SURFACE ACTIVE)

=> d l11 ibib kwic 1-
YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y


L11  ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:          2004:356124  CAPLUS
TITLE:                     Self-association of cyclodextrins and cyclodextrin
                           complexes
AUTHOR(S):                 Loftsson, Thorsteinn; Masson, Mar; Brewster, Marcus E.
CORPORATE SOURCE:          Faculty of Pharmacy, University of Iceland, Reykjavik,
                           IS-107, Iceland
SOURCE:                    Journal of Pharmaceutical Sciences (2004), 93(5),
                           1091-1099
                           CODEN: JPMSAE; ISSN: 0022-3549
```

PUBLISHER: Wiley-Liss, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB **Cyclodextrins** are useful **functional** excipients, which are being used in an ever-increasing way to camouflage undesirable pharmaceutical characteristics, especially poor aqueous solubility It has generally been assumed that the mechanism whereby cyclodextrins exert their effects, especially their augmentation of solubility, is via the formation of noncovalent, dynamic inclusion complexes. This is a model, which regards drug-cyclodextrin interactions as a discrete phenomenon and ignores the possible interaction of these complexes with one another. It is becoming increasingly apparent that such assumptions may not be universally applicable or all encompassing. Specifically, there is a growing body of evidence that supports the important contribution of non-inclusion-based aspects for drug solubilization by cyclodextrins including **surfactant**-like effects and mol. aggregation. This short review attempts to assess the available literature for areas in which such non-inclusion mechanisms are apparent and tries to interpret these in the context of a broader working theory as to how cyclodextrins exert their beneficial effects.

L11 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:570517 CAPLUS
DOCUMENT NUMBER: 113:170517
TITLE: Use of **cyclodextrin** as a **functional** food material
AUTHOR(S): Hara, Kozo
CORPORATE SOURCE: Ensuiko Seito K. K., Japan
SOURCE: Japan Fudo Saiensu (1990), 29(1), 33-41
CODEN: JAFSAA; ISSN: 0368-1122
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Japanese

TI Use of **cyclodextrin** as a **functional** food material

AB A review with 43 refs. on various applications of cyclodextrin in food products (e.g. as deodorizer, drying agent, and **emulsifier**), the absorption and metabolism of cyclodextrin in animals, and the effect of dietary cyclodextrin on rats.

L11 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:434512 CAPLUS
DOCUMENT NUMBER: 109:34512
TITLE: Studies on functional properties and applications of β-cyclodextrin. 1. Emulsification, reduction of bitterness, hygroscopicity and foaming
AUTHOR(S): Chiu, C. P.; Lin, T. C.; Cheng, S. W.; Chuang, W. L.
CORPORATE SOURCE: Dep. Nutr. Food Sci., Fn Jen Univ., Taiwan
SOURCE: Jiemian Kexue Huizhi (1988), 11(1), 38-44
CODEN: CMKCEW; ISSN: 1026-325X
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

ST **cyclodextrin functional** property application; **emulsifier** cyclodextrin; hygroscopicity cyclodextrin; foaming cyclodextrin; bitterness redn cyclodextrin

IT 7585-39-9, β- **Cyclodextrin**
RL: PROC (Process)
(**functional** properties and applications of)

=> s cyclodextrin (p) bind? (p) (surfactant)
25338 CYCLODEXTRIN

```
          8293 CYCLODEXTRINS
         26033 CYCLODEXTRIN
                 (CYCLODEXTRIN OR CYCLODEXTRINS)
       1048108 BIND?
        159739 SURFACTANT
        143359 SURFACTANTS
        202420 SURFACTANT
                 (SURFACTANT OR SURFACTANTS)
L12         100 CYCLODEXTRIN (P) BIND? (P)  (SURFACTANT)

=> s cyclodextrin (p) bind? (p)  (surfactant) (p) (interaction or affinity)
          25338 CYCLODEXTRIN
           8293 CYCLODEXTRINS
          26033 CYCLODEXTRIN
                 (CYCLODEXTRIN OR CYCLODEXTRINS)
       1048108 BIND?
        159739 SURFACTANT
        143359 SURFACTANTS
        202420 SURFACTANT
                 (SURFACTANT OR SURFACTANTS)
        809376 INTERACTION
        531978 INTERACTIONS
       1139848 INTERACTION
                 (INTERACTION OR INTERACTIONS)
        262241 AFFINITY
         32034 AFFINITIES
        277278 AFFINITY
                 (AFFINITY OR AFFINITIES)
L13          25 CYCLODEXTRIN (P) BIND? (P)  (SURFACTANT) (P) (INTERACTION OR
                AFFINITY)

=> d l13 ibib kwic 1-
YOU HAVE REQUESTED DATA FROM 25 ANSWERS - CONTINUE? Y/(N):y


L13  ANSWER 1 OF 25  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2003:1011647  CAPLUS
DOCUMENT NUMBER:          140:183140
TITLE:                    Basic Hydrolysis of Crystal Violet in
                          β-Cyclodextrin/Surfactant Mixed Systems
AUTHOR(S):                Garcia-Rio, L.; Leis, J. R.; Mejuto, J. C.;
                          Navarro-Vazquez, A.; Perez-Juste, J.;
                          Rodriguez-Dafonte, P.
CORPORATE SOURCE:         Departamento de Quimica Fisica, Facultad de Quimicia,
                          Universidad de Santiago de Compostela, Santiago de
                          Compostela, Spain
SOURCE:                   Langmuir (2004), 20(3), 606-613
                          CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
REFERENCE COUNT:          56    THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
AB   The basic hydrolysis of crystal violet (CV) in mixed systems consisting of
     β- cyclodextrin (β-CD) and a micelle-forming
     surfactant, cetyltrimethylammonium chloride (CTACl), was studied.
     β-CD catalyzes the basic hydrolysis of CV through the
     interaction of its hydroxyl group, in its deprotonated form, with
     the carbocation in the complexed substrate.  The addition of small amts. of
     CTACl, with [CTACl] below the critical micelle concentration, to β-CD solns.
     does not have an effect upon the observed rate constant for the basic
     hydrolysis of CV.  This behavior is different from that observed for the
alkaline
```

hydrolysis of N-methyl-N-nitroso-p-toluenesulfonamide and nitrophenyl acetates in mixed β-CD/cationic **surfactant** systems. The proposed mechanism explains the exptl. results on the basis of the high percentage of uncomplexed β-CD in equilibrium with the micellar system, the low CV concentration, and the high value for the **binding** constant of CV by β-CD.

L13 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:615226 CAPLUS
TITLE: Injectable nanoparticles for in vivo remediation of overdosed toxins
AUTHOR(S): Partch, Richard
CORPORATE SOURCE: Department of Chemistry, Engineering Research Center, Clarkson University, University of Florida, Potsdam, Gainesville, NY, 13699-5814, USA
SOURCE: Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States, August 18-22, 2002 (2002), COLL-238. American Chemical Society: Washington, D. C.
CODEN: 69CZPZ
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Three different approaches are being taken to prepare nanoparticles for **binding** and deactivating various chems. that cause thousand of deaths each year if accidentally or intentionally overdosed. The three therapeutics under consideration are an antiarrythmic, an antidepressant and a local anesthetic. Also of interest to detoxify are overdosed "street" drugs like cocaine, and chemical warfare agents. The three types of nanoparticles under investigation are 1) nanoemulsion dispersed phases, 2) solid particles with pores templated in size and shape for a toxin to enter, and 3) solid particles with covalently attached receptors on their surfaces having unique capability to interact with one or more of the toxins being evaluated. Resp., their modes of action can be categorized as 1) adsorption into oil, 2) adsorption inside particles, and 3) surface adsorption on particle. Furthermore, toxin destruction after capture may be facilitated by incorporation of an enzyme expressed to have enhanced oxidation of a toxin. Biocompatible oil-in-water nanoemulsions stabilized by various combinations of co-**surfactants** are employed for drug delivery. In the present research, their oil cores are proving to be excellent reservoirs for absorbing and holding lipophilic toxins. Examples of how the oil and **surfactant** compns. can be engineered to achieve selective toxin removal from blood will be described. Syntheses for porous, templated nanoparticles are well known and procedures are being adapted to create ones having enhanced adsorption (zeolite-like) properties for the toxins under consideration. The general procedure is to include mol. mimics of the toxins in the sol-gel reactions, followed by their removal after the nanoparticles are formed. The pores show some specificity in capturing molecularly similar chems. Two types of mol. receptors are being covalently attached to surfaces of both biocompatible metal oxide or organic polymer nanoparticles. One type functions by p acceptor-p donor **interaction** between the bound receptor and the toxin. The second type involves complexation of the lipophilic toxin inside a bound **cyclodextrin**. In summary, several types of chemical engineered nanoparticle systems for saving lives from overdoses of lipophilic therapeutic or "street" drug toxins have been successfully prepared The astounding ability of each to function as desired will be discussed. This presentation will focus on surface modification processes to achieve the titled goal.

L13 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:585827 CAPLUS
DOCUMENT NUMBER: 137:262738
TITLE: Thermodynamic Evidence of Cyclodextrin-Micelle

Interactions

AUTHOR(S): De Lisi, R.; Milioto, S.; Muratore, N.
CORPORATE SOURCE: Dipartimento di Chimica Fisica, Universita di Palermo, Palermo, 90128, Italy
SOURCE: Journal of Physical Chemistry B (2002), 106(35), 8944-8953
CODEN: JPCBFK; ISSN: 1520-6106
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The enthalpy of transfer (ΔHt) of hydroxypropyl-α-**cyclodextrin** (HP-α-CD), hydroxypropyl-β-**cyclodextrin** (HP-β-CD), and β- **cyclodextrin** (β-CD) from water to the aqueous C6F13CO2Na and C7F15CO2Na solns. were determined in the pre- and post-micellar regions. The behavior of the macrocycles is system specific. Generally, the magnitude of the enthalpy is influenced by several factors: (1) the alkyl chain length of the **surfactant**, (2) the **cyclodextrin** cavity and its alkylation, (3) the **interactions** between the free **cyclodextrin** and the free **surfactant**, (4) the host-guest equilibrium constant, (5) the host/guest stoichiometry, and (6) the micelle-**cyclodextrin** (free and/or complexed) **interactions**. As far as the premicellar region is concerned, HP-α-CD does not form the host-guest complexes. β-CD and HP-β-CD in the aqueous C7F15CO2Na solns. form host-guest complexes of 1:1 stoichiometry; β-CD shows a larger **binding affinity** toward the **surfactant** as a compensative effect between the more neg. enthalpy and entropy. Besides 1:1 complexes, HP-β-CD in aqueous C6F13CO2Na solns. forms complexes of 1:2 stoichiometry (1 **cyclodextrin**:2 **surfactants**). Their presence was evidenced by the min. in the ΔHt vs the **surfactant** concentration (fSmS) trend. The equation derived to take into account both 1:1 and 1:2 complexes equilibrium was successfully applied to the present data and those of HP-α-CD/sodium alkanoate systems previously studied by us. As far as the postmicellar region is concerned, HP-α-CD was treated like an additive, which distributes between the aqueous and the micellar phases. An equation was proposed to rationalize the enthalpy data dealing with the **cyclodextrins** exhibiting inclusion complex formation. It was based on the following phenomena: (1) formation of 1:1 and 1:2 complexes in the aqueous phase, (2) distribution of free **cyclodextrin**, 1:1 complex, and 1:2 complex between the aqueous and the micellar phases, and (3) shift of the micellization equilibrium induced by the **cyclodextrin**. As a general feature, **cyclodextrin** (free and/or complexed) shows **affinity** toward the micelles because of the favorable **interactions** between the carboxylate head in the hydrophilic shell and the hydroxyl groups of the **cyclodextrin**. C6F13CO2Na micelles compared to C7F15CO2Na exhibit a slightly larger **affinity** toward HP-α-CD controlled by more neg. enthalpy and entropy changes. A single mechanism governs the **interaction** between the C7F15CO2Na micelles and the 1:1 complexes of HP-β-CD/ **surfactant** and β-CD/ **surfactant**, as the standard free energy, enthalpy, and entropy of transfer of the two complexes from the aqueous to the micellar phases are identical. The 1:2 complex (1 HP-β-CD:2 C6F13CO2Na) weakly **binds** to the micelles according to the unfavorable **interactions** between the micellar surface and the doubly charged complex.

IT Micellization
(**binding** constant; thermodn. evidence of **cyclodextrin** -micelle inclusion and micellization **interactions** involving perfluoroalkanoate **surfactants**)

L13 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:578608 CAPLUS
DOCUMENT NUMBER: 137:376674
TITLE: Inclusion complexation of (11-ferrocenylundecyl)trimethylammonium bromide by β-cyclodextrin and its effects on electrochemical behavior of the surfactant
AUTHOR(S): Komura, T.; Yamaguchi, T.; Noda, K.; Hayashi, S.
CORPORATE SOURCE: Faculty of Engineering, Division of Material Chemistry, Kanazawa University, Kanazawa, 920-8667, Japan
SOURCE: Electrochimica Acta (2002), 47(20), 3315-3325
CODEN: ELCAAV; ISSN: 0013-4686
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB This report describes the influence of β- **cyclodextrin** complexation on thermodn. and kinetic parameters of the electrode reaction of (11-ferrocenylundecyl)trimethylammonium bromide in aqueous media. The host attracted the reduced form having a less pos. charge more strongly than the corresponding oxidized one. Thus, a hydrophobic **interaction** between the non-polar host cavity and the ferrocene moiety plays an important role in the inclusion complexation. Fast-scan voltammetric behavior of the amphiphilic ion suggested that inclusion-ejection processes practically attain equilibrium in the scan-rate range below 10 V s-1, because of their fast rates. The relation between the peak current and peak potential leads to the conclusion that the enveloped guest exchanges no electrons directly with an electrode. The mean diffusion coefficient of the **surfactant** can be written as a linear combination of the contributions from a free monomol., a micelle-forming, and a host-bound **surfactant**. Since the **binding affinity** of the ferrocene moiety for the host cavity is much stronger than the aggregation force between the amphiphilic mols. in aqueous media, the host disrupts the micelles by incorporating the **surfactant** mol. into its cavity.

L13 ANSWER 5 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:550155 CAPLUS
DOCUMENT NUMBER: 137:268776
TITLE: Studies on interaction of β-cyclodextrin with amphoteric surfactant
AUTHOR(S): Zhang, You-ming; Peng, Xiao-xia; Wei, Tai-bao; Wang, Han-qing
CORPORATE SOURCE: Department of Chemistry, Northwest Normal University, Lanzhou, 730070, Peop. Rep. China
SOURCE: Wuji Huaxue Xuebao (2002), 18(8), 773-776
CODEN: WHUXEO; ISSN: 1001-4861
PUBLISHER: Wuji Huaxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The inclusion complexes of β- **cyclodextrin** (β-CD) with amphoteric **surfactants** (C11H23CONHCOONa, SF) in aqueous solns. have been studied by surface tension measurement at different temps. The surface tension curves of the **surfactants** in the presence of β-CD are higher than that in the absence of β-CD. The curves raise higher with the increase of β-CD concns. of **surfactant** . The apparent critical micelle concentration (cmc) of the **surfactant** varies linearly with β-CD concentration The inclusion consts. (Ka) of the inclusion complexes were determined by surface tension at different temps. The Ka decreases with the increase of temperature In addition, the standard molar Gibbs energies, enthalpies, entropies were derived for the **interaction**

process by Ka at different temps. The results indicated that the association of **surfactants** with β-CD are favorable by both enthalpy and entropy changes, proving that hydrophobic **interaction** was the dominant **binding** force of the **cyclodextrin** inclusion complex.

L13 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:829673 CAPLUS
DOCUMENT NUMBER: 136:124021
TITLE: Interaction of sulfonated ruthenium(II) polypyridine complexes with surfactants probed by luminescence spectroscopy
AUTHOR(S): Garcia-Fresnadillo, David; Orellana, Guillermo
CORPORATE SOURCE: Dept. de Quimica Organica, Facultad de Ciencias Quimicas, Universidad Complutense de Madrid, Madrid, E-28040, Spain
SOURCE: Helvetica Chimica Acta (2001), 84(9), 2708-2730
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB Novel anionic [RuL2L']2- complexes, where L stands for (1,10-phenanthroline-4,7-diyl)bis(benzenesulfonate) (pbbs) or (2,2'-bipyridine)-4,4'-disulfonate (bpds), and L' is N-(1,10-phenanthrolin-5-yl)tetradecanamide (pta) or N-(1,10-phenanthrolin-5-yl)acetamide (paa), were synthesized, and their **interaction** with the prototypical **surfactants** sodium dodecylsulfate (SDS), cetyl tri-Me ammonium bromide (CTAB), and Triton X-100 (TX-100) was investigated by electronic absorption, luminescence spectroscopy, emission-lifetime detns., and O2-quenching measurements. [Ru(pbbs)2(pta)]2- (I) displayed cooperative self-aggregation in aqueous medium at concns. above 1.3 μM; the observed association was enhanced in the presence of either β- **cyclodextrin** or NaCl. This amphiphilic RuII compound showed the strongest **interaction** with all the detergents tested: nucleation of **surfactant** mols. around the luminescent probe was observed below their resp. critical micellar concns. As much as a 12-fold increase of the emission intensity and a 3-fold rise in the lifetime were measured for I bound to TX-100 micelles; the other complexes showed smaller variations. The O2-quenching rate consts. decreased up to 1/8 of their original value in H2O (e.g., for [Ru(bpds)2(pta)]2- bound to CTAB micelles). Luminescence-lifetime expts. in H2O/D2O allowed the determination of the metal-complex fraction exposed to solvent after **binding** to **surfactant** micelles. For instance, such exposure was as low as 25% for pta complexes·CTAB aggregates. The different behaviors observed were rationalized in terms of the RuII complex structure, the electrostatic/hydrophobic **interactions**, and the probe environment.

L13 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:293098 CAPLUS
DOCUMENT NUMBER: 133:17192
TITLE: Multiple Complexation of Didecyldimethylammonium Bromide and Cyclodextrins Deduced from Electromotive Force Measurements
AUTHOR(S): Funasaki, Noriaki; Neya, Saburo
CORPORATE SOURCE: Kyoto Pharmaceutical University, Kyoto, 607-8414, Japan
SOURCE: Langmuir (2000), 16(12), 5343-5346
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The 1:1 and 1:2 macroscopic **binding** consts. of didecyldimethylammonium bromide (DDAB) and α-, β-, and γ-**cyclodextrins** (CD) are determined from the electromotive force measurements with a DDAB-selective electrode, and the magnitude of these consts. is interpreted in terms of the mol. structures of complexes. The 1:1 macroscopic **binding** consts. of a double chain **surfactant** is 2-fold larger than that of a single chain, because the former has two chains. The 1:1 macroscopic **binding** consts. of DDAB are in the increasing order γ-CD < α-CD ≈ β-CD, consistent with those of a single chain **surfactant**. In the 1:1 complex of DDAB and γ-CD, one or two decyl chains are incorporated into the CD cavity. The 1:2 macroscopic **binding** consts. of DDAB are in increasing order γ-CD « β-CD « α-CD. This order is interpreted in terms of the structure of complexes: the first larger ligated CD inhibits the second ligation more strongly. The present result serves for the quant. understanding of the **interaction** between membrane phospholipid and CD as well as the structure-complexation relationship.

L13 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:83946 CAPLUS
DOCUMENT NUMBER: 132:199387
TITLE: Thermodynamic investigation (volume and compressibility) of the systems β-cyclodextrin + n-alkyltrimethylammonium bromides + water
AUTHOR(S): Gonzalez-Gaitano, G.; Crespo, A.; Tardajos, G.
CORPORATE SOURCE: Departamento de Quimica y Edafologia (seccion de Quimica Fisica) Facultad de Ciencias, Universidad de Navarra, Pamplona, 31080, Spain
SOURCE: Journal of Physical Chemistry B (2000), 104(8), 1869-1879
CODEN: JPCBFK; ISSN: 1089-5647
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB D. and sound velocity data for aqueous solns. at 298 K containing a homolog series of alkyltrimethylammonium bromides (CnTAB, n = 10, 12, 14, 16) in the absence and presence of β- **cyclodextrin** were analyzed to calculate the molar apparent and partial vols. and adiabatic compressibilities. For the binary systems, the molar partial compressibilities and vols. of the pure **surfactants** in water were obtained as a function of the concentration and compared with the literature data, and the methylene group contributions were deduced. For the ternary systems, a remarkable increase of both the molar partial volume and compressibility of the **surfactant** at infinite dilution with respect to the value in water is observed The large values of the transfer properties of the **surfactants** at infinite dilution, molar partial compressibilities and vols., can be discussed in terms of a simple model in which the balance between the released water from the cavity and the methylene groups of the substrate that enter into the macrocycle is considered. The pos. molar compressibility of the **surfactant** when it is forming the complex, compared to the neg. value when it is in pure water, proves the hydrophobic component of the **interaction**. Both partial molar volumes and compressibilities of the **surfactants** are the same in the absence and in the presence of

β-CD at high **surfactant** molalities, indicating the nonparticipation of the complex into the micelles, and the CMCs are displaced in an extension that shows the participation of a 2:1 stoichiometry with the longest homologues (n = 14, 16). The application of Young's rule permits to calculate the reaction parameters from the bibliog. data of the **binding** consts. The transfer vols. and compressibilities increase with n, indicating that the predominant stoichiometry turns to 2:1 when the hydrocarbon chain is long enough.

L13 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:680609 CAPLUS
DOCUMENT NUMBER: 132:40888
TITLE: Molar Partial Compressibilities and Volumes, 1H NMR, and Molecular Modeling Studies of the Ternary Systems β-Cyclodextrin + Sodium Octanoate/Sodium Decanoate + Water
AUTHOR(S): Gonzalez-Gaitano, G.; Sanz-Garcia, T.; Tardajos, G.
CORPORATE SOURCE: Departamento de Quimica-Fisica I Facultad de Quimicas, Universidad Complutense, Madrid, 28040, Spain
SOURCE: Langmuir (1999), 15(23), 7963-7972
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The thermodn. behavior of the ternary systems β- **cyclodextrin** (β-CD) + Na octanoate (NaO) or Na decanoate (NaD) + H2O was studied from d. and speed of sound measurements in a broad concentration range at 298 K and at natural pH. The molar partial compressibilities and vols. of the pure **surfactants** in H2O as a function of concentration were obtained and compared with the literature data. For the ternary systems, a remarkable increase of the molar partial compressibility of the **surfactant** at infinite dilution with respect to the value of the **surfactant** in H2O is observed, whereas it does not change in the micelle region, and the same behavior is found with the partial volume The changes in the transfer properties of the **surfactants** at infinite dilution, molar partial compressibilities, and vols. can be discussed in terms of a simple model in which it is considered the balance between the released H2O from the cavity and the methylene groups of the substrate that enter into the macrocycle. The pos. molar compressibility of the **surfactant** when it is forming the complex, as a difference with the neg. value when it is in pure H2O, prove the hydrophobic component of the **interaction** and permits estimating from this property the **binding** consts. by application of Young's rule. 1H NMR studies on the systems permit one to elucidate the complex structure and corroborate the thermodn. data. The association consts. and stoichiometry were deduced from vols., compressibilities, and 1H NMR data, yielding consistent values that agree with other literature results obtained at fixed pH. Mol. mechanics calcns. were performed to shed light on the structure of the complex in solution The results confirm the NMR data and indicate that the polar head in the complex is at the wider rim of the macrocycle, protruding in the cavity, with the **surfactant** tilted within the β-CD.

L13 ANSWER 10 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:738343 CAPLUS
DOCUMENT NUMBER: 130:116695
TITLE: Interaction of Triton X-100 with cyclodextrins. A fluorescence study
AUTHOR(S): Datta, Anindya; Mandal, Debabrata; Kumar Pal, Samir; Das, Swati; Bhattacharyya, Kankan
CORPORATE SOURCE: Department of Physical Chemistry, Indian Association

for the Cultivation of Science, Jadavpur, Calcutta, 700 032, India
SOURCE: Journal of the Chemical Society, Faraday Transactions (1998), 94(23), 3471-3475
CODEN: JCFTEV; ISSN: 0956-5000
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The **interaction** of Triton X-100 (TX) with α- and β-**cyclodextrins** (CD) was studied, using 2,6-p-toluidinonaphthalene sulfonate (TNS) as a fluorescent probe, by steady-state and time-resolved emission spectroscopy. The critical micellar concentration (c.m.c.) is indicated by the point of abrupt increase of emission intensity and lifetime of TNS. The apparent c.m.c. increases significantly in the presence of β-CD by ≤28 ± 1 times at 10 mM β-CD but remains more or less unaffected in the presence of α-CD at similar concns. This is attributed to the very strong **binding** of TX with the large β-CD cavity and negligible **binding** to the small α-CD. At concns. below the c.m.c., on addition of TX to aqueous TNS solution containing β-CD the emission intensity decreases. This is ascribed to the competitive **binding** of TNS and TX with β-CD. This causes displacement of TNS from the CD cavity by the TX **surfactant** mols. The **binding** constant of TX with β-CD is .apprx.9400 ± 1300 L mol-1.

L13 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:690020 CAPLUS
DOCUMENT NUMBER: 130:78408
TITLE: Microcalorimetry of Chiral Surfactant-Cyclodextrin Interactions
AUTHOR(S): Cooper, Alan; Nutley, Margaret A.; Camilleri, Patrick
CORPORATE SOURCE: Chemistry Department, Glasgow University, Glasgow, G12 8QQ, UK
SOURCE: Analytical Chemistry (1998), 70(23), 5024-5028
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The **interactions** of the chiral **surfactants** taurodeoxycholate (TDOCA) and deoxycholate (DOCA) with a range of **cyclodextrins** in aqueous solution have been investigated by isothermal titration microcalorimetry. In the presence of β- **cyclodextrin**, the apparent critical micelle concentration (cmc) of taurodeoxycholate is increased, and the enthalpy of demicellization decreased, in a manner consistent with 1:1 complexation of TDOCA with β-CD at low concns. There is no evidence for direct **interaction** of **cyclodextrins** with **surfactant** micelles. This is confirmed by more direct **binding** titrns. Below the cmc, TDOCA forms 1:1 host-guest complexes with β- **cyclodextrin** (ΔH.degree .**bind** = -32 kJ mol-1, Kdiss = 0.38 mM; 25°, pH 7), methyl-β- **cyclodextrin** (ΔHbind = -13 kJ mol-1, Kdiss = 0.36 mM), hydroxypropyl-β- **cyclodextrin** (ΔH.degree .**bind** = -12 kJ mol-1, Kdiss = 0.51 mM), and γ- **cyclodextrin** (ΔH.degree .**bind** = -7.3 kJ mol-1, Kdiss = 0.08 mM), but not with the smaller α-**cyclodextrin**. At higher **cyclodextrin** concns., the calorimetric **binding** data are more ambiguous, suggesting 2:1

cyclodextrin/TDOCA complexation. Similar results are found with DOCA, though expts. here are limited by the tendency of DOCA to form gels in aqueous buffers. Enhanced chromatog. or electrophoretic chiral resolution observed in mixed chiral **surfactant/cyclodextrin** phases could be the result of increased solubility and/or the multiplicity of chiral complexes in such systems.

L13 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:628136 CAPLUS
DOCUMENT NUMBER: 129:307121
TITLE: Study of surfactant-cyclodextrin complexation by cyclic voltammetry using polypyridyl metal complexes as electroactive probes
AUTHOR(S): Raj, C. Retna; Ramaraj, R.
CORPORATE SOURCE: School of Chemistry, Madurai Kamaraj University, Madurai, 625 021, India
SOURCE: Electrochimica Acta (1998), 44(2-3), 279-285
CODEN: ELCAAV; ISSN: 0013-4686
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB Polypyridyl ruthenium(II) and cobalt(III) complexes were chosen as electroactive probes to study **surfactant-cyclodextrin** (CD) complexation. The complexation of sodium dodecyl sulfate (SDS) with CD and its influence on the electrochem. of these metal complexes were studied. Complexation of SDS with CD released the metal complex from the SDS **interaction**. The ratio of Kred/Kox (ratio of **binding** consts. of reduced and oxidized forms of the metal complex) decreased upon the addition of CD and it confirmed the elimination of the **interaction** between SDS and metal complex and the inclusion of SDS into the cavity of CD. The insol. precipitate formed at lower concentration of SDS with polypyridyl ruthenium(II) complex was solubilized by the addition of CD and is due to the inclusion of SDS into the cavity of CD. The SDS mol. prefers to **bind** with CD rather than with the metal complex. Geometric constraint forbid the inclusion of polypyridyl metal complex into the cavity of CDs. The critical micellar concentration (cmc) of SDS increased with increasing the concentration of β-CD. The electrochem. of metal complexes has not been altered by the SDS-CD inclusion complex. The [CD] required to break the **surfactant interaction** has been determined by cyclic voltammetry. The emission spectral study also confirmed the release of metal complex from the **surfactant interaction** upon the addition of CD.

L13 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:491177 CAPLUS
DOCUMENT NUMBER: 129:246883
TITLE: 19F and 1H NMR Investigation of Cyclodextrin/Fluorocarbon Alkyl Carboxylate Surfactant Inclusion Complexes
AUTHOR(S): Wilson, L. D.; Verrall, R. E.
CORPORATE SOURCE: Department of Chemistry, University of Saskatchewan, Saskatoon, SK, S7N 5C9, Can.
SOURCE: Langmuir (1998), 14(17), 4710-4717
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB A 19F NMR chemical shift study of a homologous series of perfluorocarbon (fc)

[CxF2x+1CO2Na, x = 3, 4, 6-9] **surfactants** (S) has been carried out in D2O and in binary solvent (D2O + **cyclodextrin** (CD)) systems at 22 °C. Both β-CD and modified **cyclodextrins** were used. Complementary 1H NMR chemical shift data for the **cyclodextrins** in binary solvent (D2O + S) systems were also obtained. Values of the complex-induced chemical shifts (CIS) for selected host or guest nuclei are observed to increase with increasing alkyl chain (Cx) length of the **surfactant** when the CD/S complex has a 1:1 stoichiometry. However, for complexes having stoichiometries other than 1:1 CD/S, somewhat different trends in the CIS values were observed **Binding** consts. (Ki) have been obtained from the anal. of 19F and 1H CIS values of the CD/S systems using equilibrium models in which 1:1, 1:1 plus 2:1, 1:1 plus 1:2 complexes, and uncomplexed species are present. In general, Ki increases as Cx increases; however, differences in the **binding affinity**, stoichiometry, and inclusion geometry of the CD/S complexes were observed to depend on the type of **cyclodextrin**. The latter can be understood in terms of the steric effects created by the introduction of alkyl groups in the annulus region of the **cyclodextrin**.

L13 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:263809 CAPLUS
DOCUMENT NUMBER: 129:4796
TITLE: A 1H NMR study of cyclodextrin - hydrocarbon surfactant inclusion complexes in aqueous solutions
AUTHOR(S): Wilson, Lee D.; Verral, Ronald E.
CORPORATE SOURCE: Department of Chemistry, University of Saskatchewan, Saskatoon, SK, S7N 5C9, Can.
SOURCE: Canadian Journal of Chemistry (1998), 76(1), 25-34
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB A 1H NMR chemical shift (δ) study of a homologous series of hydrocarbon (hc) (CxH2x+1CO2Na, x = 5, 7, 9, 11, 13) **surfactants** (S) has been carried out in water and in binary solvent (D2O + **cyclodextrin** (CD)) systems at 22°C. Complementary 1H NMR chemical shift (δ) data of the **cyclodextrins** in binary (D2O + S) systems containing hc **surfactants** have also been obtained. Complex induced shift (CIS) values for selected host or guest protons were found to increase as the alkyl chain (Cx) length of the **surfactant** increased. The CIS values are found to depend on the following factors: (i) the magnitude of the **binding** constant (Ki, i = 1:1, 2:1), (ii) the chain length of the **surfactant**, (iii) the mole ratio of the host to guest species, (i.v.) the host-guest stoichiometry, and (v) the host-guest inclusion geometry. The CIS values of the CD-S systems have been analyzed using equilibrium models in which 1:1 complexes, 1:1 plus 2:1 complexes, and uncomplexed species are present. Differences in the **binding affinity**, stoichiometry, and inclusion geometry of the complexes formed between a given hc **surfactant** and the various **cyclodextrins** were observed

L13 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:45122 CAPLUS
DOCUMENT NUMBER: 128:90328
TITLE: Volumetric Study of Modified β-Cyclodextrin/Hydrocarbon and /Fluorocarbon Surfactant Inclusion Complexes in Aqueous Solutions
AUTHOR(S): Wilson, Lee D.; Verrall, Ronald E.
CORPORATE SOURCE: Department of Chemistry, University of Saskatchewan, Saskatoon, SK, S7N 5C9, Can.

SOURCE: Journal of Physical Chemistry B (1998), 102(2), 480-488
CODEN: JPCBFK; ISSN: 1089-5647
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The apparent molar volumes (Vϕ,S) of homologous series of hydrocarbon (hc) [CxH2x+1CO2Na, x = 5, 7, 9, 11, 13] and perfluorocarbon (fc) [CxF2x+1CO2Na, x = 3, 6-9] **surfactants** (S) have been determined in water and in binary solvent (H2O + modified β- **cyclodextrin** (R-β-CD)) systems at 25 °C. The apparent molar volumes (Vϕ,R-β-CD) of 2,6-di-O-methyl-β-CD (DM-β-CD) and 6-(2-hydroxypropyl)-β-CD (HP-β-CD) in water and in binary (H2O + S) systems containing hc and fc **surfactants** have also been obtained. The magnitudes of Vϕ,S and Vϕ,R-β-CD are greater in ternary solns. than in the binary aqueous systems. The apparent molar volumes of the modified **cyclodextrins** and the **surfactants** at infinite dilution ($V^{\circ}\phi$) in ternary solns. depend on the following factors: the magnitude of the **binding** constant (Ki), the alkyl chain length of the **surfactant**, the mole ratio of the host to guest species, the nature of the host/guest stoichiometry, and the physicochem. properties of the CD and/or the **surfactant**. The volumetric properties of the ternary systems have been analyzed in terms of the additive contributions of the complexed and uncomplexed species. R-β-CD/ **surfactant** complexes having 1:1 and 1:1 plus 1:2 stoichiometries were successfully modeled using two-site and three-site equilibrium models, resp. The **binding affinities** of hc and fc **surfactants** with DM-β-CD and HP-β-CD show different behavior.

L13 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:611539 CAPLUS
DOCUMENT NUMBER: 127:248371
TITLE: Steric control for the hydrolysis of enantiomeric and diastereomeric esters. A new development of supramolecular assemblies
AUTHOR(S): Goto, Kouichi; Ueoka, Ryuichi
CORPORATE SOURCE: Grad. Course Appl. Chem., Kumamoto Inst. Technol., Kumamoto, 860, Japan
SOURCE: Yuki Gosei Kagaku Kyokaishi (1997), 55(9), 803-813
CODEN: YGKKAE; ISSN: 0037-9980
PUBLISHER: Yuki Gosei Kagaku Kyokai
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Japanese

AB A review with 49 refs. The remarkably high enantioselectivity (kLa,obsd/kDa,obsd = 1000) was attained for the hydrolysis of amino acid esters [N-dodecanoyl-D(L)-phenylalanine p-nitrophenyl ester; C12-D(L)-Phe-PNP] catalyzed by the active tripeptide [N-(benzyloxycarbonyl)-L-phenylalanyl-L-histidyl-L-leucine; Z-Phe-His-Leu] in the coaggregate systems composed of 41 mol% hexadecyltrimethylammonium bromide (CTAB) and 59 mol% ditetradecyldimethylammonium bromide (2C14Br) at the specific ionic strength (μ = 0.02). With respect to the temperature dependence of hydrolysis in the coaggregate systems composed of native lipid (L-α-dipalmitoylphosphatidylcholine; DPPC) and nonionic **surfactant** [α-[4-(1,1,3,3-tetramethylbutyl)phenyl]-ω-hydroxydecakis(oxyethylene); Triton X-100], the enantioselectivity was maximized at the phase transition temperature (Te) and the hydrophobic microenvironment of coaggregates could be evaluated on the basis of isokinetic temperature (β). On the other hand, in the stereoselective hydrolysis of dipeptide esters as mediated by **cyclodextrins** (CyD), a high diastereoselectivity (kDL2/kLL2 = 46) and preferential

binding property (KDLb/KLLb = 2.4) were observed for the hydrolysis of N-(benzyloxycarbonyl)-D(L)-phenylalanyl-L-phenylalanine p-nitrophenyl ester (Z-D(L)-Phe-L-Phe-PNP) by γ-CyD. Furthermore, the computer modeling (MOPAC calcn.) study suggests that a favorable mol. recognition between the substrate and catalyst through the effective hydrophobic **interactions** and hydrogen bonds should be very important for the enhancement of stereoselectivity.

L13 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:579575 CAPLUS
DOCUMENT NUMBER: 127:248302
TITLE: A spectral displacement study of the binding constants of cyclodextrin-hydrocarbon and -fluorocarbon surfactant inclusion complexes
AUTHOR(S): Wilson, Lee D.; Siddall, Stephanie R.; Verrall, Ronald E.
CORPORATE SOURCE: Department of Chemistry, University of Saskatchewan, Saskatoon, SK, S7N 5C9, Can.
SOURCE: Canadian Journal of Chemistry (1997), 75(7), 927-933
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The preparation of title **cyclodextrin** inclusion complexes with hydrocarbon and fluorocarbon carboxylate is reported. The spectral displacement technique with phenolphthalein as the chromophore has been used to obtain 1:1 equilibrium **binding** consts. (K2) for a homologous series of hydrocarbon (hc) ($C_nH_{2n+1}COONa$, n = 5-13) and fluorocarbon (fc) anionic **surfactants** ($C_nF_{2n+1}COONa$, n = 3-8) with β-**cyclodextrin** (β-CD). The magnitude of K2 increases as the alkyl chain length increases in each homologous series. K2 values in the ranges of 102-105M-1 and 101-104M-1 were obtained for the β-CD-fc and for the β-CD-hc **surfactant** complexes, resp. The different **binding affinity** of β-CD with hydrocarbon and -fluorocarbon **surfactants** is discussed in terms of such physicochem. properties of the guest species as hydrophobicity, geometrical size, conformational effects, mol. polarizability, and solvation of the head group.

L13 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:549669 CAPLUS
DOCUMENT NUMBER: 125:329163
TITLE: Conductivity studies of the molecular encapsulation of sodium perfluoroctanoate by β-cyclodextrin derivatives
AUTHOR(S): Junquera, Elena; Pena, Lourdes; Aicart, Emilio
CORPORATE SOURCE: Dep. Quim. Fisica I, Univ. Complutense Madrid, Madrid, 28040, Spain
SOURCE: Journal of Inclusion Phenomena and Molecular Recognition in Chemistry (1996), 24(3), 233-239
CODEN: JIMCEN; ISSN: 0923-0750
PUBLISHER: Kluwer
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The mol. encapsulation of sodium perfluoroctanoate (SPFO) by hydroxypropyl-β- **cyclodextrin** (HP-β-CD) or 2,6-di-O-methyl-β- **cyclodextrin** (DM-β-CD) has been analyzed by measuring the conductivity in solution of the ternary systems formed by CD + SPFO + H_2O. The studies were carried out at 25°C using a fully computerized elec. conductivity technique. The measurements were made as a

function of CD concentration at various non-micellar concns. of SPFO, and as a function of CD and SPFO concns. with [CD]/[SPFO] constant at stoichiometric ratio. The inclusion complexes, HP-β-CD-SPFO and DM-β-CD SPFO, were characterized through the stoichiometry, which has been found to be 1:1 in both cases, and the **binding** consts., which have been evaluated from the conductivity data with a model proposed by us considering the variation of the ionic molar conductivities with the concentration and the association of the **surfactant** counter-ion to the inclusion complex. The resulting K values indicate that the **interaction** between the CD cavity and the monomeric SPFO is strong and similar in both cases.

L13 ANSWER 19 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:460337 CAPLUS
DOCUMENT NUMBER: 125:166930
TITLE: Selectivity in the binding and detection of charge diffuse ions
AUTHOR(S): Parker, David; Kataky, Ritu; Kelly, Patricia M.; Palmer, Simon
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK
SOURCE: Pure and Applied Chemistry (1996), 68(6), 1219-1223
CODEN: PACHAS; ISSN: 0033-4545
PUBLISHER: Blackwell
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with .apprx.30 refs. The selective **binding** of charge diffuse alkyl and arylammonium ions relies upon multiple weak **interactions** with a complementary synthetic receptor. Using appropriately sized lipophilic **cyclodextrin** derivs., the chemoselective **binding** of alkylammonium ions such as dopamine, acetylcholine, guanidine, and long chain cationic **surfactants** may be achieved allowing their selective detection by either potentiometric or amperometric methods of anal. Enantioselectivity in the **binding** of chiral β-hydroxyarylammonium ions, such as propranolol, allows chiral sensors to be developed. The selective detection of various clin. important analytes, such as imipramine, lignocaine and creatinine has also been studied.

L13 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:121718 CAPLUS
DOCUMENT NUMBER: 124:219419
TITLE: Quantitative structure-activity relationship studies with micellar electrokinetic chromatography. Influence of surfactant type and mixed micelles on estimation of hydrophobicity and bioavailability
AUTHOR(S): Yang, Shenyuan; Bumgarner, Jefferson G.; Kruk, Lisa F. R.; Khaledi, Morteza G.
CORPORATE SOURCE: North Carolina State University, Department of Chemistry, Raleigh, NC, 27695-8204, USA
SOURCE: Journal of Chromatography, A (1996), 721(2), 323-35
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Applications of micellar electrokinetic chromatog. (MEKC) in quant. structure-activity relationships (QSAR) were studied. First, quant. structure-retention relationships (QSRR), which describe the correlation between logarithm of capacity factor (log k') in MEKC and logarithm of distribution coefficient between 1-octanol and water (log Pow), were investigated for 60 aromatic compds. and 9 corticosteroids using three different anionic **surfactants** [e.g., sodium dodecyl sulfate (SDS), sodium cholate (SC), and lithium perfluorooctane sulfonate (LiPFOS)], one cationic **surfactant** (C14TAB), and mixed anionic

micellar systems. Linear solvation energy relationships (LSER) and solvatochromic parameters were used to shed light on the different log k' vs. log Pow relationships for the various **surfactants**. It was concluded that hydrogen bonding **interactions** have a great influence on retention behavior in MEKC and its relationship with hydrophobicity. Interestingly, bile salt **surfactants** (e.g., SC) and mixed bile salt micellar systems provide better correlations for log k' vs. log Pow than SDS and/or SDS with buffer additives (e.g., β-**cyclodextrin**, urea, and acetonitrile). Using SC micelles, only one line was adequate to describe the relationship between retention in MEKC and hydrophobicity for a group of 60 aromatic compds. The existence of higher correlation for the SC system was attributed to a similar hydrogen bonding pattern between SC micelles and 1-octanol. In the SDS system, however, three lines were recognized for the congeneric subgroups of compds. This is due to the hydrogen bond donor (HBD) characteristic of SDS micelles that selectively differentiate between the solutes with different hydrogen bond acceptor (HBA) strength, thus demonstrating that retention is not solely based on hydrophobicity. A similar result was observed for a C14TAB-MEKC system, however, the HBA characteristic of C14TAB selectively differentiates between the solutes with different HBD strength. In addition, quant. retention-activity relationships in MEKC were also investigated for 9 corticosteroids. Two types of biol. activities [small intestinal absorption in the rat (log A/NA) and protein **binding** to human serum albumin (log B/F)] were examined in this work. High correlations were observed between bioactivity and log k' in MEKC using bile salt **surfactants** and mixed bile salt systems.

L13 ANSWER 21 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:530804 CAPLUS
DOCUMENT NUMBER: 119:130804
TITLE: Simultaneous chiral separation of leucovorin and its major metabolite 5-methyltetrahydrofolate by capillary electrophoresis using cyclodextrins as chiral selectors: estimation of the formation constant and mobility of the solute-cyclodextrin complexes
AUTHOR(S): Shibukawa, A.; Lloyd, D. K.; Wainer, I. W.
CORPORATE SOURCE: Dep. Oncol., McGill Univ., Montreal, QC, H3G 1Y6, Can.
SOURCE: Chromatographia (1993), 35(7-8), 419-29
CODEN: CHRGB7; ISSN: 0009-5893
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Capillary electrophoresis with an electrolyte containing **cyclodextrin** was investigated for the simultaneous separation of the diastereoisomers of 6R,S-leucovorin and its active metabolite 6R,S-5-methyltetrahydrofolate. α, β And γ- **cyclodextrin** separated the diastereomers of 5-methyltetrahydrofolate, while only γ- **cyclodextrin** was found to be effective for the chiral separation of leucovorin. The effect of γ- **cyclodextrin** concentration was investigated, and subsequently a curve-fitting anal. for the quant. estimation of the **binding** consts. was attempted. The **binding** consts. were found to be very small, in the range 2-4 M-1. Although the **interaction** between γ-**cyclodextrin** and the tetrahydrofolates is weak, the high efficiency of capillary electrophoresis and the use of high concns. of γ- **cyclodextrin** allow baseline chiral separation of the diastereoisomers of leucovorin and 5-methyltetrahydrofolate. Changes in temperature exert differing effects on the sepns. of leucovorin and 5-methyltetrahydrofolate; higher temps. improved the separation of leucovorin diastereoisomers but reduced the resolution of 5-methyltetrahydrofolate diastereomers. The effects of urea and buffer salt concns. and of buffer pH were also investigated. Capillary electrophoresis with γ-**cyclodextrin** was used to analyze plasma samples spiked with clin.-relevant levels of leucovorin and 5-methyltetrahydrofolate. Resolution of these compds. in filtered plasma was demonstrated, but detection

sensitivity was not adequate for the routine use of this method for the determination of leucovorin and 5-methyltetrahydrofolate in plasma. In addition, a simple technique to reverse the elution order of ionic stereoisomers was demonstrated. By adding a cationic **surfactant** into the buffer and reversing the separation potential, the elution order of the diastereoisomers of leucovorin and 5-methyltetrahydrofolate was reversed.

L13 ANSWER 22 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:537565 CAPLUS
DOCUMENT NUMBER: 117:137565
TITLE: Binding of dibenzepine to cyclodextrins and anionic surfactants in aqueous solution
AUTHOR(S): Gonzalez-Blanco, Carmen; Moro, Manuel E.; Mercedes Velazques, M.; Rodriguez, Licesio J.
CORPORATE SOURCE: Fac. Farm., Univ. Salamanca, Salamanca, E-37080, Spain
SOURCE: Farmaco (1992), 47(5), 623-30
CODEN: FRMCE8; ISSN: 0014-827X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The **binding** of dibenzepine to α-, β-, and γ-**cyclodextrins**, and to the anionic **surfactants**: sodium octyl, decyl, dodecyl and tetradecyl sulfates, in aqueous solution, has been studied by a UV spectrophotometric technique. A particular dependence on **cyclodextrin** cavity size and on **surfactant** hydrocarbon chain length is evident from the obtained results. The **binding affinity** follows the trend: β- > γ- > α-**cyclodextrin**; tetradecyl > dodecyl > decyl > octyl sulfate.

L13 ANSWER 23 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:480440 CAPLUS
DOCUMENT NUMBER: 109:80440
TITLE: Effect of hydrophobic-lipophilic **interactions** on chemical reactivity. III. Contributions of hydrophobic **interactions** to the **binding** of fluorocarbon **surfactants** by β- **cyclodextrin** and of lipophilic **interactions** to the **binding** of hydrocarbon substrates by amylose-type hosts [Erratum to document cited in CA108(12):101682c]
AUTHOR(S): Jiang, Xikui; Gu, Jianhua; Cheng, Xianen; Hui, Yongzheng
CORPORATE SOURCE: Shanghai Inst. Org. Chem., Acad. Sin., Shanghai, Peop. Rep. China
SOURCE: Huaxue Xuebao (1988), 46(2), 206
CODEN: HHHPA4; ISSN: 0567-7351
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
TI Effect of hydrophobic-lipophilic **interactions** on chemical reactivity. III. Contributions of hydrophobic **interactions** to the **binding** of fluorocarbon **surfactants** by β-**cyclodextrin** and of lipophilic **interactions** to the **binding** of hydrocarbon substrates by amylose-type hosts [Erratum to document cited in CA108(12):101682c]

L13 ANSWER 24 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:101682 CAPLUS
DOCUMENT NUMBER: 108:101682
TITLE: Effect of hydrophobic-lipophilic **interactions** on chemical reactivity. III. Contributions of hydrophobic **interactions** to the **binding** of fluorocarbon **surfactants** by β- **cyclodextrin** and of lipophilic

interactions to the **binding** of hydrocarbon substrates by amylose-type hosts

AUTHOR(S): Jiang, Xikui; Gu, Jianhua; Cheng, Xianen; Hui, Yongzheng

CORPORATE SOURCE: Shanghai Inst. Org. Chem., Acad. Sin., Shanghai, Peop. Rep. China

SOURCE: Huaxue Xuebao (1987), 45(2), 159-65
CODEN: HHHPA4; ISSN: 0567-7351

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

TI Effect of hydrophobic-lipophilic **interactions** on chemical reactivity. III. Contributions of hydrophobic **interactions** to the **binding** of fluorocarbon **surfactants** by β-**cyclodextrin** and of lipophilic **interactions** to the **binding** of hydrocarbon substrates by amylose-type hosts

AB With **cyclodextrin** (α- and β-CD) and Na carboxymethylamylose (Na-CMA) substrates, and with H(CF2)12CO2K, CH3(CH2)10CO2K, Cl(CF2)8CH2CH2N+Me3I- (I), CH3(CH2)8CH2N+Me3I- (II), Cl(CF2)10CH2CH2N+Me3I- and CH3(CH2)10CH2N+Me3I- (III) as guests, the different behaviors of fluorocarbon and hydrocarbon **surfactants** were studied by surface tension measurements. Limited cavity size prevents the inclusion of fluorocarbon **surfactants** by α-CD, but the **binding** by β-CD is stronger for the fluorocarbon (I) than that for its hydrocarbon analog (II). A comparison of the thermodn. parameters of the β-CD **binding** process for (I) and (III) reveals that for the former the **binding** process is driven by entropy or hydrophobic forces, but for the latter the process is enthalpy-favored. Notably, Na-CMA fails to **bind** the fluorocarbons. A crucial difference between the **cyclodextrins** and the amylose-type hosts lies in the fact that the former possess pre-organized cavities whereas the latter have to readjust their conformations from loose and extended helices with random coils to interrupted helices during the process of **binding**. Apparently, this extra energy requirement demands contributions from lipophilic **interactions** for accomplishment which do not exist between fluorocarbon chains and the hosts. Thus lipophilic forces are significant in hydrophobic-lipophilic **interactions**.

L13 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:73345 CAPLUS

DOCUMENT NUMBER: 106:73345

TITLE: Luminescence probes for the investigation of the structure and dynamics of aqueous solutions of micelles and related systems

AUTHOR(S): Turro, Nicholas J.

CORPORATE SOURCE: Dep. Chem., Columbia Univ., New York, NY, USA

SOURCE: Report (1986), ARO-19800.13-CH; Order No. AD-A169161/7/GAR, 7 pp. Avail.: NTIS
From: Gov. Rep. Announce. Index (U. S.) 1986, 86(21), Abstr. No. 646,661

DOCUMENT TYPE: Report; General Review

LANGUAGE: English

AB Among the important results discovered by this research are (1) the ability of luminescence probes to determine the nature and extent of **binding** of substrates to **cyclodextrins**; (2) the use of fluorescence probes to determine critical micelle concns., to reveal **surfactant**/polymer **interactions**; (3) the utility of fluorescence probes for investigation of non-ionic **surfactants** and of ionic/non-ionic **surfactant interactions**; (4) the ability of fluorescence probes to investigate the **interactions** of metals and **surfactant** crown ethers; (5) the use of phosphorescence metal complexes to study the nature of metal **binding** to DNA; (6) the utility of fluorescence probes to reveal

temperature and pressure effects on the properties of water soluble block co-polymers; (7) the ability of fluorescence probes to elucidate the nature and mechanisms of cation formation and proton transfer in aqueous systems. Finally, an extensive review of photochem. reactions in micelles is given.

ST luminescence probe micelle structure dynamics; **binding** substrate **cyclodextrin** luminescence probe; **surfactant** micellization fluorescence probe; polymer **surfactant** **interaction** fluorescence probe; metal **surfactant** **interaction** fluorescence probe; DNA metal **binding** fluorescence probe; photochem reaction micelle fluorescence review

=> d his full

(FILE 'HOME' ENTERED AT 19:08:59 ON 24 JUN 2004)

FILE 'CAPLUS' ENTERED AT 19:09:29 ON 24 JUN 2004

L1 137 SEA ABB=ON PLU=ON (UNATTACHED OR UNCOMPLEX OR NON-COMPLEXED OR FREE OR UNBOUND) (2A) CYCLODEXTRIN

L2 11 SEA ABB=ON PLU=ON L1 (P) (SURFACTANT OR EMULSIFIER OR SURFACE ACTIVE)

L3 285707 SEA ABB=ON PLU=ON Y
D L2 IBIB KWIC 1-

L4 32 SEA ABB=ON PLU=ON (UNATTACHED OR UNCOMPLEX OR NON-COMPLEXED OR FREE OR UNBOUND) (A) CYCLODEXTRIN

L5 5 SEA ABB=ON PLU=ON L4 (P) (SURFACTANT OR EMULSIFIER OR SURFACE ACTIVE)
D L5 IBIB KWIC 1-

L6 78 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN

L7 0 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN (3A) (FREE OR UNBOUND OR UNCOMPLEXED OR UNATTACHED)

L8 0 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN (P) (FREE OR UNBOUND OR UNCOMPLEXED OR UNATTACHED)

L9 2 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN (P) (SURFACTANT OR EMULSIFIER OR SURFACE ACTIVE)

L10 2 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN (P) (SURFACTANT OR TENSIDE OR EMULSIFIER OR SURFACE ACTIVE)
D L9 IBIB KWIC 1-
D L9 IBIB KWIC 2

L11 3 SEA ABB=ON PLU=ON FUNCTIONAL (2A) CYCLODEXTRIN AND (SURFACTANT OR TENSIDE OR EMULSIFIER OR SURFACE ACTIVE)
D L11 IBIB KWIC 1-

L12 100 SEA ABB=ON PLU=ON CYCLODEXTRIN (P) BIND? (P) (SURFACTANT)

L13 25 SEA ABB=ON PLU=ON CYCLODEXTRIN (P) BIND? (P) (SURFACTANT) (P) (INTERACTION OR AFFINITY)
D L13 IBIB KWIC 1-

FILE HOME

FILE CAPLUS

FILE COVERS 1907 - 24 Jun 2004 VOL 140 ISS 26
FILE LAST UPDATED: 23 Jun 2004 (20040623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> log h

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	230.84	231.05

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-24.26	-24.26

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 19:19:19 ON 24 JUN 2004